N-(1-Naphthyl)ethylenediamine 551-09-7 | DTXSID7043744

Model Performance

Mode	Data

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

Model Results

Predicted value: 1.87

Global applicability domain: Inside

Local applicability domain index: 6.19e-01

Confidence level: 6.68e-01

Nearest Neighbors from the Training Set

Image not found

1-Nitroso-4-phenylpiperidine

Measured: 2.59 Predicted: 1.80

Image not found

Benzylamine, p-chloro-N-methyl-

N-nitroso-**Measured:** 2.19

Predicted: 1.56

Image not found

N-Nitroso-N-(4-

bromobenzyl)methylamine

Measured: 1.57 Predicted: 1.61